Improved Description of One- and Two-Hole Excitations after Electron Capture in 163 Holmium and the Determination of the Neutrino Mass.

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Abstract

The atomic pair ^{163}Ho and ^{163}Dy seems due to the small Q value of about 2.5 keV the best case to determine the neutrino mass by electron capture. The bolometer spectrum measures the full deexcitation energy of Dysprosium (by X rays and Auger electrons plus the recoil of Holmium, which can be neglected). The spectrum has an upper limit given by the Q value minus the neutrino mass. Till now this spectrum has been calculated allowing in Dysprosium excitations with 3s1/2, 3p1/2, 4s1/2, 4p1/2, 5s1/2, 5p1/2 (and 6s1/2) holes only. Robertson [R. G. H. Robertson, arXiv: 1411.2906v1] calculated recently also the spectrum with two electron hole excitations in Dy. He took the probability for the excitation for the second electron hole from work of Carlson and Nestor [T. A. Carlson, C. W. Nestor, T. C. Tucker, and F. B. Malik, Phys. Rev. 169, 27 (1968); T. A. Carlson and C. W. Nestor, Phys. Rev. A8, 2887 (1973)] for Z=54 Xenon. The neutrino mass must finally be obtained by a simultaneous fit together with the Q value and the properties of the relevant resonances for the upper end of the spectrum. Under the assumption only one resonance (independent of its nature: one-, two-, multi-hole or of other origin,) near the Q value determines the upper end of the spectrum, and the profile of this leading state is Lorentzian, one has to fit simultaneously four parameters (neutrino mass, strength, distance of the leading resonance to the Q value and its width). If more than one resonance are of comparable importance for the upper end of the spectrum, it might be difficult or even impossible to extract the neutrino mass reliably. Compared to the work of Robertson this work includes the following improvements: (1) The two hole probabilities are calculated in the Dirac-Hartree-Fock (DHF) approach in Holmium and Dysprosium and not in Xenon. (2) In calculating the probability for the second electron hole in Dysprosium the n s1/2 or n p1/2 ($n \geq 3$) one hole states are included selfconsistently in the DHF iteration. (3) Since Dysprosium has Z=66 electrons and Xenon only Z=54, one has at least 8 additional two hole states, which do not exist in Xenon and thus their probabilities have not been calculated by Carlson and Nestor and not been included by Robertson. They are included here. (4) For the probabilities of the one hole states, which determine the main structure of the spectrum, the overlap and exchange corrections are taken into account. (5) In solving the DHF electron wave functions the finite size of the nuclear charge distribution is included. (6) The nuclear matrix elements for electron capture integrates the charge of the captured electron over the nucleus with the weight $\psi(r)^2_{e,n,\ell,j} \cdot r^2$. For the capture probability thus the value $\psi^2_{e,n,\ell,j}(R) \cdot R^2$ is taken at the nuclear radius and not the value $\psi^2_{e,n,\ell,j}(r = 0.0)$ *at* $r = 0.0$, which has the weight r^2 zero. (7) The formulas are derived in second quantization including automatically the antisymmetrization.

1 Introduction

The determination of the absolute value of the neutrino masses is one of the most important open problems in particle physics. Presently major efforts are underway to measure in the single beta decay, specifically in the Tritium decay, the electron antineutrino mass (KATRIN) [1]. The neutrinoless double beta decay can distinguish between Dirac and Majorana neutrinos and is in principle able to measure the effective Majorana neutrino mass [2]. Electron capture measures the electron neutrino mass [3, 4, 5, 6]. The sensitivity to the electron neutrino mass is increased (as in the single beta decay) in electron capture by a smaller Q value. Perhaps the best system for the determination of the absolute scale of the electron neutrino mass (and with the help of neutrino oscillations also of the muon and tauon neutrinos) by electron capture is the system ${}^{163}_{67}Ho$ and ${}^{163}_{66}Dy$.

The electron neutrino mass can in principle be determined by the upper end of the deexcitation (bolometer) spectrum of ${}^{163}Dy$ after electron capture in ${}^{163}Ho$. All deexcitation spectra (X rays, Auger electron and the recoil of Holmium) end at the Q value (for ${}^{163}Ho$ around 2.5 keV, see section 2 for the present Q value situation) minus the neutrino mass.

Recently Robertson [7] included in the atomic excitations of Dysprosium also a second hole. The deexcitation bolometer spectrum including also the two-hole states adds to the leading contributions of the one-hole spectrum a "fine structure". For the probability of the second hole in Z=66 Dy Robertson used results of Carlson and Nestor [8, 9] determined in Z=54 Xenon.

The neutrino mass must be obtained by a simultaneous fit of the Q value and the neutrino mass to the upper end of the spectrum including also properties of one-hole, two-hole and other excitations close to Q. This complicates the neutrino mass determination. In case, that several resonances determine the upper end of the spectrum this can make the determination of the neutrino mass even impossible. If only one resonance determines the upper end of the spectrum and the line profile is Lorentzian, one has to fit four parameters: neutrino mass, the distance of the leading resonance to the Q value, the strength, and the width. Before one fits the the theoretical spectrum to the upper end of the measurement, one has to fold the theory with the detector response including the finite resolution.

The improvements compared to the work of Robertson [7], Carlson and Nestor [8, 9] are:

- The two hole probabilities are calculated here with a fully relativistic Dirac-Hartree-Fock (DHF) code of Grant [10], Desclaux [11] and Ankudinov et al. [12] with the full antisymmetrization in the atoms Holmium and Dysprosium involved in the electron capture and not in Xenon.

- In calculating the probability for the second electron hole in Dysprosium the n s1/2 or n p1/2 ($n \geq 3$) one hole states are included selfconsistently in the DHF iteration. Thus for each one hole state in Dysprosium a full selfconsistent DHF iteration with a hole in the different one hole states is performed for all electrons in the atom. The electron wave functions in Ho and Dy for the same quantum numbers $|n, \ell, j>$ but with different holes change markedly. In a very rough approximation for a first orientation without the Pauli correction the probability for the second hole is:

$$P(two-hole) \approx [1.0 - < Ho, n, \ell, j | Dy, n, \ell, j >^{2(2j+1)}] \tag{1}$$

  The overlap of electron orbitals with the same quantum numbers in Ho and Dy are typically around 0.999 (see eq. (2) and eq. (3)). Thus a relative change in the overlap by one percent can change the two hole probability by a factor 10. Eq. (1) serves as lever to enlarge a small change or error in the overlap into a large change in the two-hole probability. Therefore the electron wave functions for the overlaps should be calculated in Holmium and Dysprosium and in

the determination of the Dy electron wave functions the one hole state must be selfconsistently included, if one wants to obtain reliable probabilities for the two-hole states.

- Since in Z=66 Dysprosium one has more electrons than in Z=54 Xenon, one has at least 8 additional two hole states (3s1/2 4f5/2; 3s1/2 4f7/2; 3p1/2 4f5/2; 3p1/2 4f7/2; 4s1/2 4f5/2; 4s1/2 4f7/2; 4p1/2 4f5/2 4p1/2 4f7/2), which do not exist in Xenon and thus their probabilities have not been calculated by Carlson and Nestor [8, 9] and have not been included by Robertson [7]. They are included here. The excitation energies of these states are according to tables 1 and 2 around 2050, 1845, 415 and 335 eV. Two hole states involving the one hole orbital 6s1/2 (P1) are not included here, because already the 5s1/2 has only an excitation energy of 44.7 eV. The 6s1/2 excitation energy is expected around 5 eV, i. e. 100 times smaller than the excitations neglected by Robertson [7]. In addition the ionization energy of the 6s1/2 state in the atoms involved seems not to be available in the literature and these very lightly bound electrons are not well described by Slater determinants due to configuration mixing.

- The electron wave functions in the parent and in the daughter atom get more and more similar with increasing charge number Z, since the relative change $\Delta Z/Z$ is smaller. Thus the overlaps of the wave functions for Z in the parent and (Z-1) in the daughter increase closer to unity and the sudden approximation yields a smaller two hole excitation probability, which is very roughly given by eq. (1). The overlaps are tabulated in Faessler, Gastaldo and Simkovic [4]. They are close to unity. Thus the change of these overlaps from Xenon to Holmium-Dysprosium needs only to be one percent to yield a difference of a factor ten or more for the two-hole probabilities. For one hole in the Dysprosium state 3s1/2 or 4s1/2 :

$$\begin{aligned} \text{hole in 3s1/2:} \quad & < Ho, 3s1/2 | Dy, 3s1/2 > = \ 0.999390; \\ & < Ho, 4s1/2 || Dy, 4s1/2 > = \ 0.999332; \end{aligned} \tag{2}$$

$$\begin{aligned} \text{hole in 4s1/2:} \quad & < Ho, 3s1/2 | Dy, 3s1/2 > = \ 0.999377; \\ & < Ho, 4s1/2 | Dy, 4s1/2 > = \ 0.998870; \end{aligned} \tag{3}$$

(All numbers in this work are calculated in double precision.)

- For the probabilities of the one hole states 3s1/2 (M1), 3p1/2 (M2), 4s1/2 (N1), 4p1/2 (N2), 5s1/2 (O1), 5p1/2 (O2), 6s1/2 (P1), which determine the main structure of the spectrum, the overlap and exchange corrections are included according to Faessler, Gastaldo and Simkovic [4].

- In solving the DHF electron wave functions [2, 10, 11, 12] the nuclear charge distribution is included by the Fermi parametrization determined by electron-nucleus scattering.

- The nuclear matrix element for electron capture integrates the charge of the captured Ho electron over the nucleus with the weight $\psi^2(r)_{e,n,\ell,j} \cdot r^2$. For the capture probability thus the value $\psi^2(R)_{e,n,\ell,j} \cdot R^2$ is taken (R = nuclear radius) and not the value $\psi^2(r = 0.0)_{e,n,\ell,j}$ at r = 0.0, which has the r^2 weight zero.

- The formulas are derived in second quantization including automatically the full antisymmetrization. This formulation allows not only to describe two-hole states but also to extend the description for three holes and even more hole states.

2 Description of Electron Capture and the Atomic Wave Functions

The bolometer spectrum of the deexcitation of ^{163}Dy after electron capture in ^{163}Ho can be expressed as [3] and [4] assuming Lorentzian line profiles:

$$\frac{d\Gamma}{dE_c} \propto \sum_{i=1,...N_\nu} (Q - E_c) \cdot U_{e,i}^2 \cdot \sqrt{(Q - E_c)^2 - m_{\nu,i}^2} \sum_{f=f'} \lambda_0 B_f \frac{\Gamma_{f'}}{2\pi} \frac{1}{(E_c - E_{f'})^2 + \Gamma_{f'}^2/4} \tag{4}$$

With $Q = 2.3$ *to* 2.8 *keV* [5, 18, 19, 21, 22], with a recommended value [20] $Q = (2.55 \pm 0.016)$ keV, $U_{e,i}^2$ the probability for the admixture of different neutrino mass eigenstates $i = 1, ..N_\nu$ into electron neutrinos and E_c is the excitation energy of final Dysprosium; B_f are the overlap and exchange corrections; λ_0 contains the nuclear matrix element squared [23]; $E_{f'}$ are the one- and two-hole excitation energies in Dysprosium; $\Gamma_{f'}$ are the widths of the one- and two-hole states in Dysprosium [4].

Here as in all other calculations for the deexcitation of Dy after electron capture a Lorentzian shape is assumed. This is probably a good description. Holmium is in the ECHo experiment built in a gold film positioned as an interstitial or it occupies a position of the gold lattice. A Gaussian shape would be expected in a gas from Doppler broadening. Even collision and pressure broadening yield usually a Lorentzian profile. But since the shape of the resonance lines are important for the determination of the neutrino mass, the line shapes should be studied in the future more carefully.

Results of the ECHo collaboration [21] yield for electron capture in ^{163}Ho to ^{163}Dy a Q-value:

$$Q(ECHo) = (2.80 \pm 0.08)\ keV. \tag{5}$$

The highest two hole state in Dy has an energy of 2.474 keV (see table 1) far below the Q value. So three-hole and multi-hole states (and perhaps also states from configuration mixing), which can be higher in energy, might be more dangerous for the determination of the neutrino mass.

We assume, that the total atomic wave function can be described by a single Slater determinant. B_f takes into account the overlap and the exchange terms between the parent $|G>$ and the daughter atom in the state $|A'_f>$ with a hole in the electron state $|f'>$. We use the sudden approximation as Faessler et al. [15]. B_f is the overlap and exchange correction for the electron capture probability from the state f relative to the capture from $3s_{1/2}$ in Ho with one hole in f' in the Dy atom, given in eq. (6) in the Vatai approximation [13, 14]. But the numerical value used here are calculated with the full overlap and exchange corrections of Faessler et al. [4].

$$B_f = \frac{|\psi_f(R) < A'_f|a_f|G > |^2}{|\psi_{3s1/2}(R)|^2} = P_f \cdot \frac{|\psi_f(R)|^2}{|\psi_{3s1/2}(R)|^2} \tag{6}$$

For two-hole final states one has to multiply eq.(6) according to (15) with the probability to form a second hole characterized by the quantum numbers "p' ". One has to replace $< A'_{f'}|a_i|G >$ by $< A'_{f',p';q'}|a_i|G >$ with the two electron holes f' and p' and the additional electron particle q' in Dysprosium above the Fermi surface F. The probability for the leading expression (Wick [16] contracted) to form one hole in Dy in f' = f = i is:

$$P_f = | < A'_{f'}|a_{i=f}|G > |^2 \approx \prod_{k=1,...Z;\neq f} | < k'|k > |^2 \tag{7}$$

The corresponding probability for two final hole states f' and p' and an additional electron in q' summed over all $q' > F$ of the unoccupied bound and the continuum states is:

$$P_{p'/f'} = \sum_{q'>F} | < A'_{f',p';q'} | a_i | G > |^2 \tag{8}$$

The antisymmetrized Slater determinants for the wave functions of the initial Holmium in the ground state $|G>$ and the excited one electron hole states $|A'_f>$ in Dysprosium read in second quantization:

$$|G> = a_1^\dagger a_2^\dagger a_3^\dagger ... a_Z^\dagger |0> \tag{9}$$

$$|A'_f> = a_1'^\dagger a_2'^\dagger ... a_{f'-1}'^\dagger a_{f'+1}'^\dagger ... a_Z'^\dagger |0> \tag{10}$$

The antisymmetrized two-hole state in Dy is:

$$|A'_{p',f'}> = a_1'^\dagger a_2'^\dagger ... a_{f'-1}'^\dagger a_{f'+1}'^\dagger ... a_{p'-1}'^\dagger a_{p'+1}'^\dagger ... a_Z'^\dagger a_{q'>F}'^\dagger |0> \tag{11}$$

The primes with the dagger indicate the single electron spinor creation operators for the daughter nucleus (Dysprosium) with one electron hole in the single particle state $|f'>$ in eq. (10) and two holes $|f'>$ and $|p'>$ in eq. (11). The following expressions have to be calculated with the help of Wick's theorem [16]. One considers the Wick contractions as an expansion with the "non-diagonal" overlaps as small parameters. The leading term is the expression without "non-diagonal" overlaps.

$$P_f = | < A'_f | a_i | G > |^2 = | < 0 | a'_Z a'_{Z-1} ... a'_{f+1} a'_{f-1} ... a'_1 \cdot a_f \cdot a_1^\dagger a_2^\dagger a_3^\dagger ... a_Z^\dagger | 0 > |^2 \tag{12}$$

$$P_{p/f} = | < A'_{p',f'} | a_f | G > |^2 = \sum_{q'>F} | < 0 | a'_{q'} a'_Z ... a'_{p'+1} a'_{p'-1} ... a'_{f+1} a'_{f-1} ... a'_1 \cdot a_f \cdot a_1^\dagger a_2^\dagger a_3^\dagger ... a_Z^\dagger | 0 > |^2 \tag{13}$$

The leading expression (without the sub-leading exchange terms, which contain at least one "non-diagonal" overlap in the amplitude) is obtained in eq. (12) for electron capture in Holmium from the state i, if the captured electron i in Ho has the same quantum numbers n, ℓ *and* j as the final hole state f' in Dy, i.e. for the quantum numbers i = f = f'. The probability for two hole states eq. (13) is next to the leading order, since it contains always at least one "non-diagonal" overlap $< q' | p >$ for the amplitude and the square for the probability. If the sequence of f' and p' is reversed in Dysprosium the Fermion creation operators produce automatically a "-" sign for the amplitude, which does not matter for the probability.

3 Derivation of the Probabilities

It has been already stressed, that the leading contribution for the one-hole state in eq. (12) and for the two hole state in eq. (13) is obtained, if the orbital quantum numbers for the captured electron in Holmium $|i> = |n, \ell, j, m>$ are the same as the hole quantum numbers in Dy $|f'> = |n', \ell', j', m'>$, thus $i = f' = f$ and $n = n'$, $\ell = \ell'$, $j = j'$ and $m = m'$.

The leading expression for the probability to excite the hole state in Dy corresponding to the quantum numbers of the state of the captured electron in Holmium is:

$$P_f = | < A'_f | a_f | G > |^2 = \prod_{k=k'<F, \neq f} < k' | k > |^2 = \prod_{(n,\ell,j)(Ho=Dy)<F_{Dy}} | < (nlj)_{Dy} | (n,\ell,j)_{Ho} > |^{2 \cdot N_{n,\ell,j}} \tag{14}$$

The definition of $N_{n,\ell,j}$ is given in eq. (23). $(n,\ell,j)_{Ho}$ and $(n,\ell,j)_{Dy}$ indicate electrons in the Ho and in the Dy atom with the same quantum numbers. Such states have a large overlap only slightly below unity.

For the following one needs some elementary laws of probability calculus:

$$P(A\ and\ B) = P(A) \cdot P(B)$$
$$P(A\ or\ B) = P(A) + P(B),\ \text{if A and B exclude each other.} \tag{15}$$

If one wants to include the leading contribution for two-holes in the final Dy atom, one must multiply expression P_f in eq. (14) with the probability $P_{p/f}$ to form an additional electron particle $q' > F; (\ F\ =$ Fermi Surface) and electron hole state $p' < F$. The excited electron q' can be in an unoccupied bound state or in the continuum of the Dy atom.

$$P_{p/f}(q' > F) = |< 0|a'_{q'}a'_Z...a'_{p'+1}a'_{p'-1}...a'_{f'+1}a'_{f'-1}...a'_{1'} \cdot a_f \cdot a_1^+...a_Z^+|0>|^2 =$$
$$|< A'_{p',f'<F;q'>F}(2\ holes)|a_f|G>|^2 \approx |< q'_{>F}|p_{<F}> \cdot \prod_{k=1..Z\neq f,p} < k'|k>|^2 \tag{16}$$

q' is an empty electron orbit in Dy, into which the electron p is scattered, and p the occupied state in Ho, from which this electron is removed. Here again k and k' and also f and f' and p and p' stand for the same electron quantum numbers $n,\ \ell,\ j$ in the parent k, f, p and the daughter atom k', f', p'. The product over k runs over occupied states $k' = k = (n_k,\ \ell_k,\ j_k,\ m_k)$ in Ho and Dy with the exemption of $f\ = (\ n_f,\ \ell_f,\ j_f,\ m_f)$. q' an empty state in Dy can be bound or in the continuum. If q' is in the continuum, one speaks of 'shake off'. Since now a "non-diagonal" overlap is involved in eq. (16) with $< q'_{Dy}|p_{Ho} >$ already in the amplitude and this expression must be squared for the probability, the two hole contributions are reduced by a "non-diagonal" overlap squared. If one exchanges the states f' and p', one obtains an additional "-" sign . But since one has to square the expression, a phase is irrelevant.

To evaluate the probability for an additional electron particle-hole state (16) one sums incoherently over all unoccupied states q'. This assumes, that the different two-hole excitations do not influence each other.

$$P_{f',p'} = \sum_{q'>F} |< p_{<F,Ho}|q'_{>F,Dy}>< q'_{>F,Dy}|p_{<F,Ho}>| \cdot \prod_{k=k'<F_{Dy}\neq f,p} |< k'_{Dy}|k_{Ho}>|^2 \tag{17}$$

Here as stressed above the sum over q' runs only over the unoccupied bound and continuum states in Dy. One can now use the completeness relation to shift the sum over q' to states away from the continuum to states, which one can calculate easier. One divides the completeness relation into two pieces: up to the last occupied state below the Fermi Surface F and all states above the last occupied state including also the continuum.

$$1 = \sum_{q'<F} < p|q'>< q'|p> + \sum_{q'>F} < p|q'>< q'|p> \tag{18}$$

The sum in eq. (17) is the last part of eq. (18) and one can transcribe (17) into:

$$P_{p/f} = \left(1 - \sum_{q'<F} < p_{Ho}|q'_{Dy}>< q'_{Dy}|p_{Ho}>\right) \prod_{k=k'<F_{Dy};\neq p,f} < k'_{Dy}|k_{Ho}> \tag{19}$$

In the literature one uses often the Vatai approximation [13, 14]: Exchange corrections have been already neglected in the previous expressions. In addition one assumes, that the overlaps of electron wave functions in the parent and the daughter atom with the same quantum numbers (given in the

product term in eq. (19)) can be approximated by unity. Typically the overlaps have values [4] $< k'_{Dy}|k_{Ho} > \approx 0.999$ and thus for Dy minus two holes $0.999^{64} \approx 0.94$. In the Vatai approximation [14] one replaces this value by 1.0.

$$P_{p/f} = \left(1 - \sum_{q'<F} < p_{Ho}|q'_{Dy} >< q'_{Dy}|p_{Ho} >\right) = \left(1 - < p_{Ho}|p'_{Dy} >< p'_{Dy}|p_{Ho} > - \sum_{q'<F, \neq p'} < p_{Ho}|q'_{Dy} >< q'_{Dy}|p_{Ho} >\right) \tag{20}$$

The physics of the two terms subtracted from 1 in eq. (20) is: The first subtracted term gives the probability, that the state p' in Dy is occupied. The second terms take into account the Pauli principle and prevent, that electrons can be moved into occupied states in Dy. The single electron states like $|p >= |n, \ell, j, m >$ include also the angular projection quantum number m. This projection is for the description of the data irrelevant. The first subtracted term in eq. (20) gives the probability, that a specific magnetic substate m' is occupied in p'. The probability, that all magnetic substates of p' are occupied is an "and" situation (15) and the probabilities for the substates have to be multiplied and one obtains the Nth. power of the single electron probability with $N_{p'} = N_{n,\ell,j;p'} = (2j+1)_{p'}$: $| < (n, \ell, j)_{p,Ho}|(n, \ell, j)_{p'.Dy} > |^{2 \cdot N_{n,\ell,j;p'}}$.

$$P_{p/f} = (1 - | < (n, \ell, j)_{p,Ho}|(n, \ell, j)_{p',Dy} > |^{2 \cdot N_{p'}} - \sum_{(n,\ell,\ j)_{q',Dy;\neq p'<F}} \frac{N_{n,\ell,j} \cdot N_{n',\ell,j}}{2j+1} | < (n, \ell, j)_{p,Ho}|(n, \ell, j)_{q',Dy} > |^2) \tag{21}$$

$$\text{for n and n' with:} \qquad N_{n,\ell,j} = 2j + 1; \tag{22}$$

But for the primary hole state f and the 4f7/2 state one has special factors:

$$N_{(n,\ell,j)_f} = 2j_f \quad and \quad N_{4f7/2} = 5. \tag{23}$$

Here $|f >$ is the orbital in Ho from which the electron is originally captured. The electron p' is moved to $4f7/2$ with now 5 electrons in this orbit to guarantee the correct number of electrons. $N_{n,\ell,j}/(2j+1)$ is the averaged probability to find an electron in the $|p, n, \ell, j, m >$ orbital and $N_{n',\ell,j}$ the number of electron in the $|q', n', \ell, j >$ state. For the probability of the second hole we used the Vatai [13, 14] approximation with the overlaps of corresponding electron wave functions with the same quantum numbers in Ho and Dy equal to unity and neglected the exchange corrections. For the "diagonal" overlaps of the order of ≈ 0.999 this is a good approximation.

- In the formation of the first hole state in orbital f in Ho and f' in Dy the electron can be captured from each projection quantum number "m". One has an "or" situation. According to eq. (15) the probabilities add up. But since one has capture only from $s_{1/2}$ and $p_{1/2}$ states, this yields a common factor two in the amplitude and thus is not relevant for the relative probabilities.

- The probability amplitude for the second hole is calculated in the sudden approximation [15] by the overlap of the ground state of Ho with the captured electron f removed with Dy with a hole in f' and the particle-hole excitation $(q'^1 \cdot p'^{-1})$. The overlap squared $| < (n, \ell, j)_{p,Ho}|(n, \ell, j)_{p'.Dy} > |^2$ gives the probability, that a specific magnetic substate $m_{p'}$ is occupied. To obtain the probability,

Table 1: One- and two-hole states in ^{163}Dy with quantum numbers n, ℓ, j. E_C is the excitation energy of the one- or the two-hole state. We adopt here for a better comparison the values for E_c and the width Γ used by Robertson in his arXiv publication [7] taken from [24], although there seem to be in some cases better values in the literature [21], [25], [26], [27] and [28]. The last two columns give the relative probabilities of the one and the two hole states in relation to $3s1/2$ in % for ^{163}Dy of the present work (P-Fae) and the publication of Robertson (P-Rob) [7]. One finds surprisingly large differences for the two-hole probabilities to Robertson [7]. To ensure, that the present values are correct, three two-hole probabilities with about the largest differences to Robertson have also been calculated by hand. The two-hole probabilities are extremely sensitive to the overlap between the relativistic electron orbitals in Ho and Dy with the same quantum numbers $|n, \ell, j >$. In a very rough approximation eq. (1) provides a lever to enlarge a small change for the overlap into a large change in the two-hole probability. The difference between the Robertson results and the present approach is largest for the outermost electron orbitals for the second hole. One expects for the slightly bound states 5s1/2, 5p1/2 and 5p3/2 for the overlaps in Xe and in Ho the largest differences, since these states are much weaker bound in Xe than in Ho. See table 3.

1. *hole*	2. *hole*	$E_c[eV]$	$\Gamma[eV]$	$P-Fae[\%]$	$P-Rob[\%]$
3s1/2	—	2041.8	13.2	100	100
3s1/2	4s1/2	2474.2	13.2	0.167	0.075
3s1/2	4p1/2	2385.3	13.2	0.103	0.11
3s1/2	4p3/2	2350.0	13.2	0.163	0.25
3s1/2	4d3/2	2201.8	13.2	0.930	1.05
3s1/2	4d5/2	2201.8	13.2	0.126	1.62
3s1/2	4f5/2	2050.4	13.2	0.165	0.0
3s1/2	4f7/2	2047.0	13.2	0.182	0.0
3s1/2	5s1/2	2091.1	13.2	0.132	1.36
3s1/2	5p1/2	2072.6	13.2	0.128	3.12
3s1/2	5p3/2	2065.9	13.2	0.185	7.31
3p1/2	—	1836.8	6	5.080	5.26
3p1/2	4s1/2	2269.2	6	0.005	0.004
3p1/2	4p1/2	2180.3	6	0.009	0.006
3p1/2	4p3/2	2145.0	6	0.007	0.014
3p1/2	4d3/2	1996.8	6	0.005	0.057
3p1/2	4d5/2	1996.8	6	0.005	0.087
3p1/2	4f5/2	1845.4	6	0.005	0.00
3p1/2	4f7/2	1842.0	6	0.012	0.00
3p1/2	5s1/2	1886.1	6	0.005	0.072
3p1/2	5p1/2	1887.6	6	0.008	0.165
3p1/2	5p3/2	1860.9	6	0.008	0.386

Table 2: Continuation of the table 1 with one and two hole states in ^{163}Dy.

1. *hole*	2. *hole*	$E_c[eV]$	$\Gamma[eV]$	$P-Fae[\%]$	$P-Rob[\%]$
4s1/2	—	409.0	5.4	24.40	23.29
4s1/2	4s1/2	841.4	5.4	0.021	0.001
4s1/2	4p1/2	752.5	5.4	0.052	0.004
4s1/2	4p3/2	717.2	5.4	0.091	0.01
4s1/2	4d3/2	569.0	5.4	0.088	0.077
4s1/2	4d5/2	569.0	5.4	0.125	0.123
4s1/2	4f5/2	417.6	5.4	0.027	0.0
4s1/2	4f7/2	414.2	5.4	0.023	0.0
4s1/2	5s1/2	458.3	5.4	0.066	0.254
4s1/2	5p1/2	439.8	5.4	0.039	0.629
4s1/2	5p3/2	433.1	5.4	0.058	1.502
4p1/2	—	328.3	5.3	1.220	1.19
4p1/2	4p1/2	671.8	5.3	0.001	0.0001
4p1/2	4p3/2	636.5	5.3	0.004	0.0005
4p1/2	4d3/2	488.3	5.3	0.005	0.004
4p1/2	4d5/2	488.3	5.3	0.006	0.006
4p1/2	4f5/2	336.9	5.3	0.002	0.0
4p1/2	4f7/2	328.3	5.3	0.001	0.0
4p1/2	5s1/2	377.6	5.3	0.002	0.013
4p1/2	5p1/2	359.1	5.3	0.004	0.031
4p1/2	5p3/2	352.4	5.3	0.002	0.076
5s1/2	5s1/2	44.7	3	3.200	3.45
5p1/2	5p1/2	21.1	3	0.157	0.15

Table 3: Ionization energies and two-hole probabilities $P[\%]$ (6) relative to the 3s1/2 state comparing Xe with Ho. A small reduction of the overlap, which is typically for well bound electron orbitals $< Z,\ n,\ \ell,\ j \mid Z-1,\ n,\ \ell,\ j > =\ 0.999$, by an assumed value of 2 % produces by the lever of eq. (1) a large increase of the second hole probability. The reduction of the overlap for going from an atom with Z to Z-1 is largest for very lightly bound electrons. The $5s1/2,\ 5p1/2\ and\ 5p3/2$ are in Xenon with Z = 54 only with half the energy E bound as in Holmium with Z = 67. The binding energies of the Holmium orbitals are taken from Robertson [7]. The values in the brackets are from the literature [24, 25, 26, 27, 28]. A decrease of the overlaps in Xenon by assumed 2 % *to* 0.979 relative to Holmium increases the probability for the second hole P(2-hole) by a factor 20. This factor increases the 2-hole probabilities in these states to roughly the values of Robertson [7] (see table 1 and 2), who used the results of Carlson and Nestor [9] calculated for Xenon. It should be stressed, that the two-hole probabilities are in this work not calculated by the very rough eq. (1) but by the more accurate expression (21).

-	$E\ [eV]\ Xenon$	$E\ [eV]\ Holmium$
$5s_{1/2}$	23.3	49.9
$5p_{1/2}$	13.4	26.3 (30.8)
$5p_{3/2}$	12.1	26.3 (24.1)
$Overlap$	$for\ (-2\ \%)$ 0.979; P(2-hole)	for 0.999; P(2-hole)
$j\ =\ 1/2$	8.1 %	0.4 %
$j\ =\ 3/2$	15.6 %	0.8 %

that all magnetic substates of p' are occupied, one has the "and" situation (15), which requires to multiply all these probabilities with each other, which yields the power of $N_{(n,\ell,j)p'}$.

- The second subtracted term in eq. (21) takes care of the Pauli principle of the occupied states apart of p'. One has an "*or*" situation. Thus one obtains a factor $N_{n,\ell,j}$ according to eqs. (15) and (23).

- The one hole f' and the particle-hole excitation $(q'^1 \cdot p'^{-1})$ are in an "and" situation. Thus the probabilities have to be multiplied $P(f'^{-1}) \cdot P(q'^1, p'^{-1})$ according to (15). One multiplies the probabilities (14) with (16). These probabilities relative to 3s1/2 (6) are listed in tables 1 and 2.

Table 4: The electron binding energies and widths of hole states in ^{163}Ho from the literature [24, 25, 26, 27, 28] and the recent ECHo data [29, 30]. Electrons below $3s_{1/2}$ can not be captured in ^{163}Ho. Due to the Q-value of about 2.8 keV they are energetically forbidden.

-	n, ℓ, j	$E_{lit}[keV]$	$E_{ECHo}[keV]$	$\Gamma_{lit}[eV]$	$\Gamma_{ECHo}[eV]$
$M1$	$3s1/2$	2.047	2.040	13.2	13.7
$M2$	$3p_{1/2}$	1.836	1.836	6.0	7.2
$N1$	$4s_{1/2}$	0.420	0.411	5.4	5.3
$N2$	$4p_{1/2}$	0.340	0.333	5.3	8.0
$O1$	$5s_{1/2}$	0.050	0.048	5.0	4.3

4 Comparison with Carlson and Nestor

Thomas A. Carlson, C. W. Nestor, Thomas C. Tucker and F. B. Malik [8, 9] derived by physics arguments for the antisymmetrization and the Pauli principle the probability to excite apart of a hole in f' also an additional particle-hole state:

$$P_{Carlson;f,p} = (1 - (| < (n,\ell,j)_{p',Dy}|(n,\ell,j)_{p,Ho} > |^2)^{N_{n\ell j}} - \sum_{n'<F;\neq n'_p} \frac{N_{n,\ell,j} \cdot N_{n',\ell,j}}{2j+1} \cdot | < n',\ell,j(Dy)|n,\ell,j(Ho) > |^2) \quad (24)$$

The definition of $N_{n,\ell,j}$ is given in eq. (23). $(n,\ell,j)_{p,Ho}$ and $(n,\ell,j)_{p',Dy}$ indicate electrons in the Ho and in the Dy atoms with the same quantum numbers.

The two expressions (21) from this paper and (24) by Carlson and Nestor [9] are in the Vatai approximation [13, 14] identical. That means one neglects exchange terms and assumes, that the overlaps of equivalent electron orbitals with the same quantum numbers in the parent and in the daughter atom are equal to unity. Thus we have in the Vatai approximation [13, 14] verified the formula of Carlson and Nestor [9] including here more rigorously the antisymmetrization and the Pauli principle and showing also expressions beyond the Vatai approximation.

The logarithmic (with basis 10) bolometer Spectrum (4) and (21) for the one and two hole probabilities of figure 1 is calculated with the parameters of Robertson [7] and a Q-value = 2.8 keV for the energy between 0.0 and 2.8 keV. In figure 2 the one-hole energies and the widths are used from table 4. The excitations of one-hole states in ^{163}Dy after electron capture in ^{163}Ho and also the excitations of two-hole states in Dy are included. For the width in this work as far as they are not known experimentally the estimates of Robertson [7] are assumed to allow a better comparison. In a linear plot of the bolometer spectrum the two hole excitations are hard to see and the spectrum calculated in this work and the one calculated with the probabilities of Robertson [7], Carlson and Nestor [9] look almost identical, although the two hole probabilities are in some cases strongly different as shown in tables 1 and 2. The two hole modifications of the bolometer spectrum show up clearly in a logarithmic plot, but are suppressed in a figure with a linear ordinate.

In figure 2 the theoretical results for the bolometer spectrum in electron capture in ^{163}Ho to ^{163}Dy of this work are compared with experimental data of Ranitzsch et al. [29] and of Gastaldo et al. [30] in a linear plot assuming a Q value of 2.8 keV.

In figure 3 the upper end (2.70 to 2.80 keV) of the theoretical linear bolometer spectrum of the present approach including one- and two-hole states are shown for an electron neutrino mass of 0.0 eV and 2 eV. A similar result is obtained for Q values Q = 2.3 keV and Q = 2.5 keV.

What happens, if the Q-value falls within the width of a two hole resonance? This situation is displayed in figure 4. The two hole resonance 3s1/2, 4p3/2 lies at 2.350 keV with a width $\Gamma = 13.2\ eV$. The figure shows the upper part of the bolometer spectrum from 2.345 to 2.355 keV for a neutrino mass of $m_\nu = 0\ eV$ and $m_\nu = 2\ eV$.

Figure 5 shows the upper end of a theoretical spectrum with a mixture of two mass eigenstates for the electron neutrino. The mixing probabilities are adopted from Capozki et al. [17]. The onset of the 10 eV admixture at 2.790 keV can be seen.

The importance of excited states in Dy for the neutrino mass determination does not depend, if it is a one-, a two- or a multi-hole state or if it is of a different nature. Under the assumption, that the shape of the resonances are Lorentzian, the importance of a specific state for the determination of the neutrino mass can be seen from eq. (4). A measure for the importance of a state for the determination of the neutrino mass is:

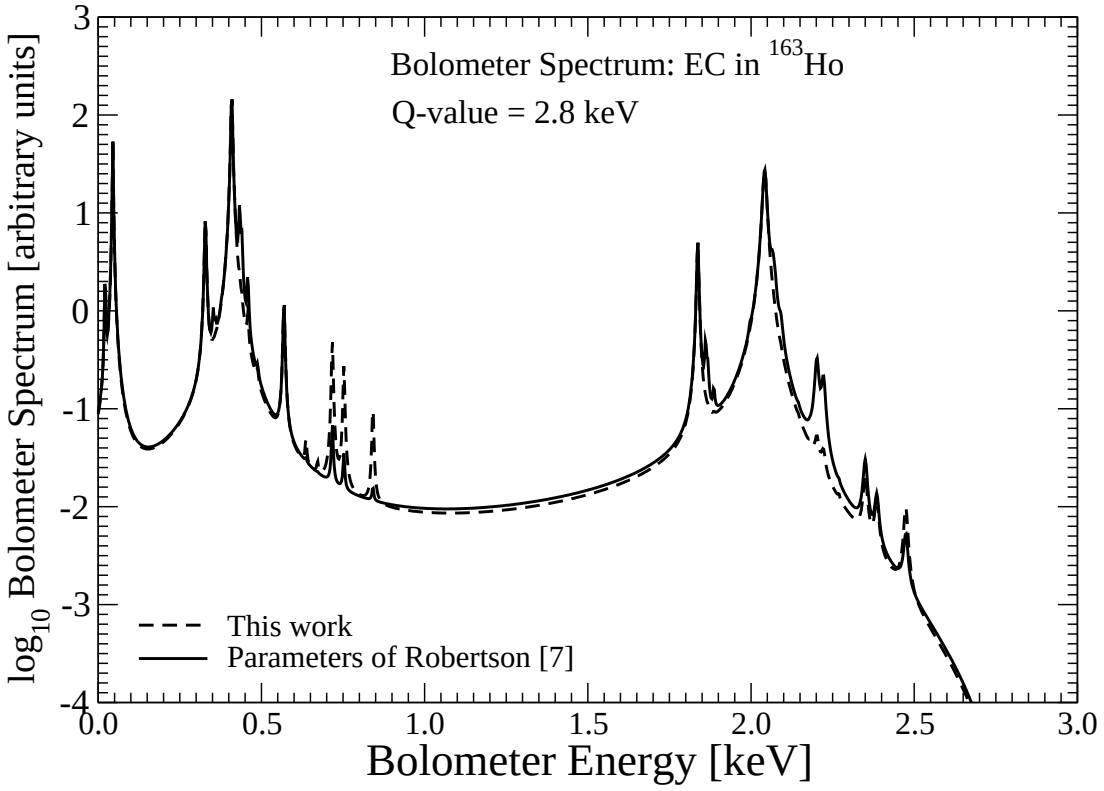

Figure 1: $Logarithmic_{10}$ (with basis 10) bolometer Spectrum (4) and (21) for the one- and two-hole probabilities calculated in this work (dashed line) and with the parameters of Robertson (solid line) [7] with the assumed Q-value = 2.8 keV for the bolometer energy between 0.0 and 2.8 keV. Apart of the excitation of one-hole states in ^{163}Dy after electron capture in ^{163}Ho also the excitations of two-hole states in ^{163}Dy are included. The $logarithmic_{10}$ plot stresses the effect of the the two hole states. In a linear plot (see figure 2) the two hole states are hardly to be seen. The values at the ordinate have to be read as $10^{ordinate}$. So "-2" is 10^{-2}.

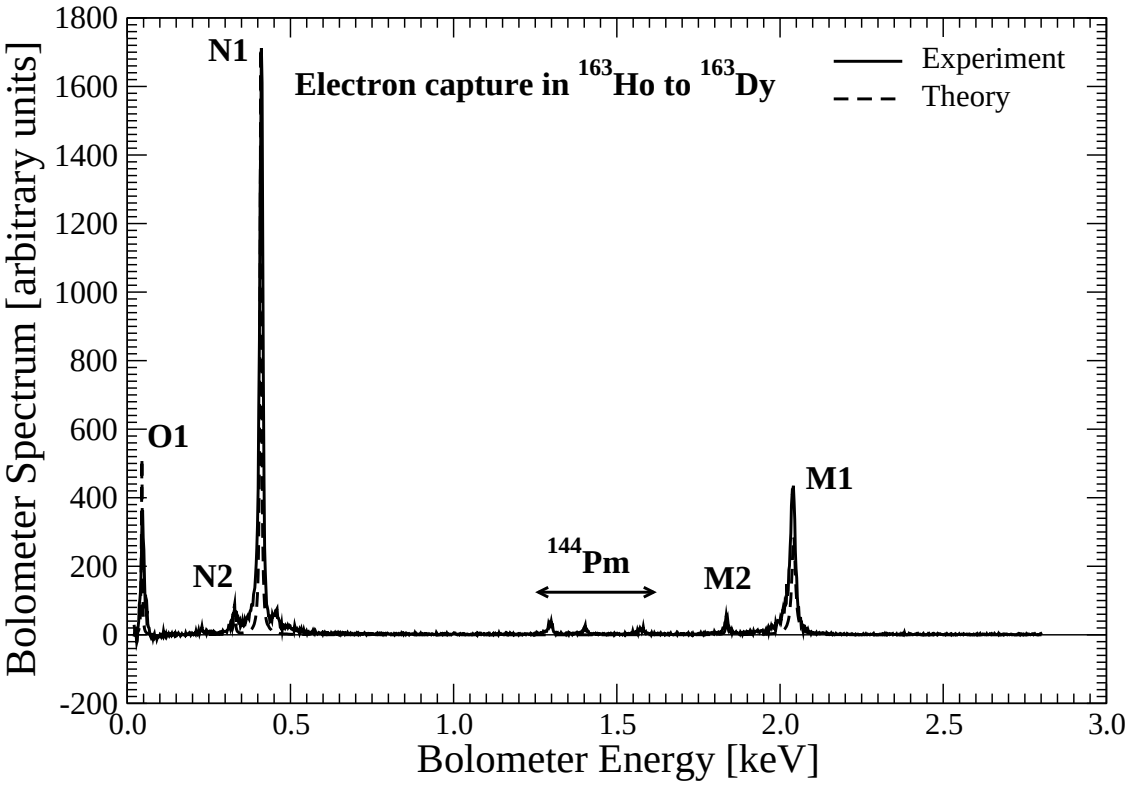

Figure 2: Experimental (solid line) and theoretical (dashed line) linear bolometer spectrum (4) and (21) for electron capture in ^{163}Ho to ^{163}Dy with the Q-value = 2.8 keV (see eq. (5)) including the one- and two-hole probabilities calculated in this work and compared to the Heidelberg experiment of Ranitzsch et al. [29] and Gastaldo et al.[30] for the total bolometer energy from 0.02 to 2.80 keV. The theoretical spectrum is normalized to the data of the N1 (4s1/2) peak at 0.42 keV. The three small experimental lines between 1.2 and 1.6 keV are originating from small admixtures of ^{144}Pm. The experimental counts are binned in 2 eV intervals. Due to background subtraction the number of counts in some bins can be negative. In some regions of the energy the number of counts per bin are zero or one. Due to negative and zero counts in a bin it is not possible to plot the data logarithmically as in figure 1, which would show the small effects of the two-hole excitations in Dy better. The theoretical spectrum is calculated for zero neutrino mass and with the excitation and width of the one hole states of the ECHo collaboration [29] and [30] listed in table 4.

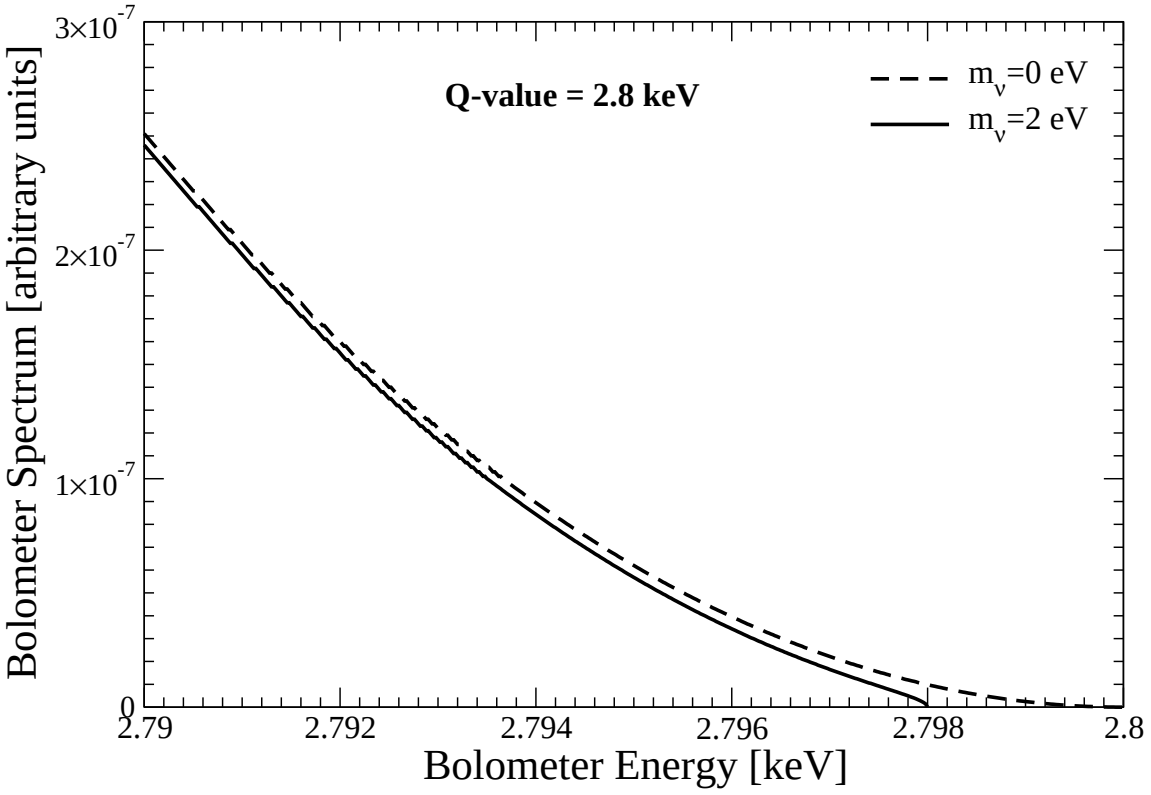

Figure 3: The upper 10 eV of the bolometer spectrum from 2.790 to the Q-value = 2.800 keV for neutrino masses $m_\nu = 0.0\ eV$ (*dashed line*) *and* $m_\nu = 2\ eV$ (*solid line*).

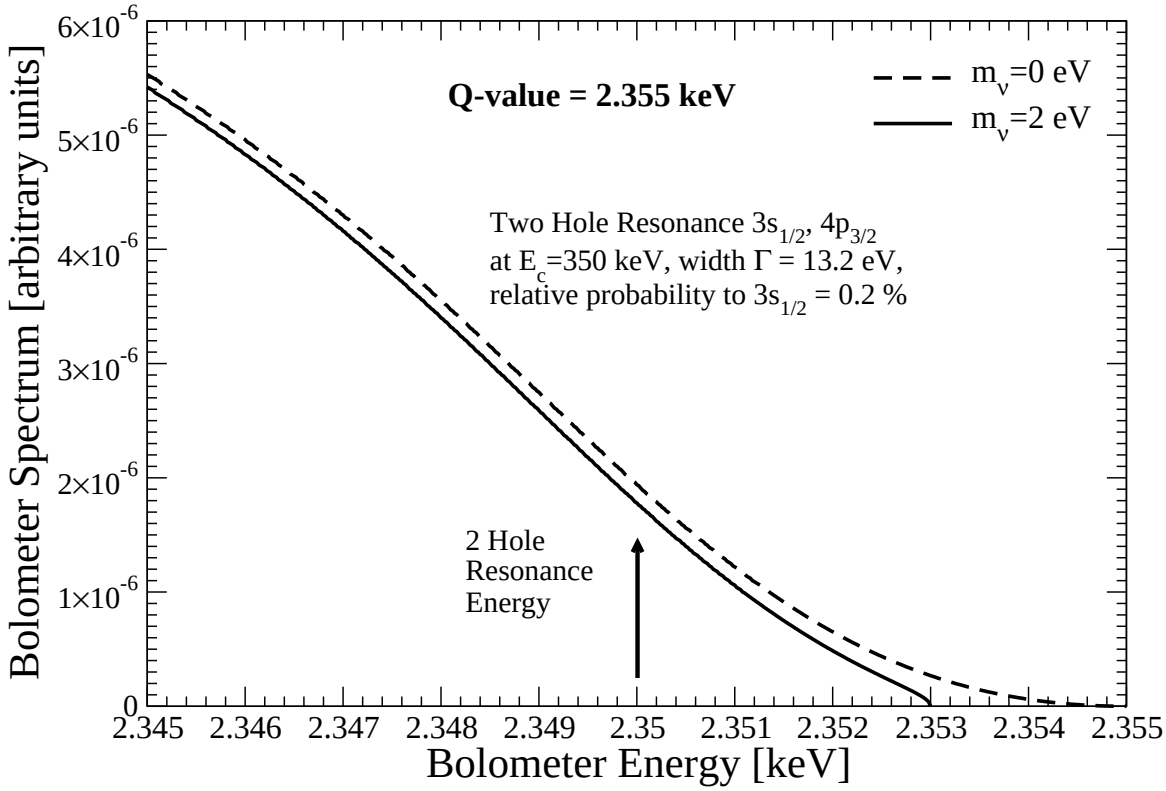

Figure 4: The upper 10 eV of the bolometer spectrum from 2.345 keV to the assumed Q-value = 2.355 keV for neutrino masses $m_\nu = 0.0\ eV$ (*dashed line*) *and* $m_\nu = 2\ eV$ (*solid line*). The two hole state $3s1/2,\ 4p3/2\ at\ E_c = 2.350\ keV$ in ^{163}Dy is just below the assumed Q-value = 2.355 keV within the width $\Gamma = 13.2\ eV$. In a simultaneous fit of the neutrino mass and the Q value also the position, the width and the strength of the resonance state must be included. A finite neutrino mass produces at the upper end of the spectrum a special fingerprint, which can not be produced by a resonance state. The fit to the upper end of the spectrum is hoped to show this fingerprint as finite neutrino mass.

$$\text{importance} \propto \frac{B_f \cdot \Gamma_{f'}}{(Q - E_{f'})^2 + \Gamma_{f'}^2/4} \approx \frac{B_f \cdot \Gamma_{f'}}{(Q - E_{f'})^2} \tag{25}$$

The dependence on the resonance energy $E_{f'}$ is $(Q - E_{f'})^{-2}$, if the distance of the energy to the Q value is larger than the width. So states near to the Q value have normally the largest influence on the determination of the neutrino mass. In general one needs a simultaneous fit of the neutrino mass, the Q value and the parameters ($E_{f'}$, $B_{f'}$ and the width $\Gamma_{f'}$) of the most important resonance (or even resonances). This makes the determination of the neutrino mass very difficult or perhaps even impossible.

To analyze how many and which parameters must be fitted to the upper end of the experimental spectrum, we introduce the definitions ΔE_C and $\Delta E_{f'}$ in eq. (26) and we assume, that only one resonance determines the upper end of the spectrum near the Q value and that the profile of this line is Lorentzian.

$$E_C = Q - \Delta E_C; \qquad\qquad E_{f'} = Q - \Delta E_{f'} \tag{26}$$

ΔE_C describes the variable energy and $\Delta E_{f'}$ the distance of the leading resonance to the Q value, and $\Gamma_{f'}$ is the width of this resonance.

$$\begin{aligned} \frac{d\Gamma}{dE_c} &\propto (Q - E_c) \cdot \sqrt{(Q - E_c)^2 - m_\nu^2} \cdot \frac{S}{(E_c - E_{f'})^2 + \Gamma_{f'}^2/4} \\ &= \Delta E_C \cdot \sqrt{\Delta E_C^2 - m_\nu^2} \cdot \frac{S}{(\Delta_{f'} - \Delta E_C)^2 + \Gamma_{f'}^2/4} \end{aligned} \tag{27}$$

Here $S \propto \lambda_0 \cdot B_f \cdot \Gamma_{f'}$ is the strength of the resonance.

An estimate shows, that the one hole states play the decisive role for the behavior at the Q value assuming, that the more accurate value of Q = 2.8 keV of the ECHo collaboration [21] is correct. The relative weight 174 for the highest one-hole state 3s1/2 at 2.0418 keV with $P_{1-hole} = 100$ % is at the Q value, the important area for the neutrino mass, by a factor 100 larger than the weight 1.6 of the highest two-hole state at 2.4742 keV with $P_{2-hole} = 0.167$ % from table 1.

$$\begin{aligned} \textit{Relative weight} &\propto \frac{P_{1-hole}\ \%}{(Q - E_{f'})^2} = \frac{100\ \%}{(2.80 - 2.04)^2} = 174 \\ \textit{Relative weight} &\propto \frac{P_{2-hole}\ \%}{(Q - E_{f'})^2} = \frac{0.167\ \%}{(2.80 - 2.47)^2} = 1.6 \end{aligned} \tag{28}$$

The widths of the one- and the two-hole states of the highest energies are assumed to be the same $\Gamma = 13.2\ eV$ (see table 1) and thus are not changing the relative weights. This means, for a Q value of Q = 2.8 keV the 2-hole states seem not to play the dominant role for the determination of the neutrino mass at least judging from the states of energies closest to the Q values.

Under the assumption, that one resonance determines the upper end of the spectrum and that the shape of this state is Lorentzian, at the Q value assuming, that the one has four parameters to fit simultaneously: the neutrino mass m_ν , the distance of the resonance to the Q value $\Delta E_{f'}$, the strength S and the width $\Gamma_{f'}$. To include the experimental resolution in the fit, one must first fold the theoretical upper end of the spectrum with the experimentally determined profile of the detector.

5 Conclusions

In the present work the bolometer spectrum after electron capture in ^{163}Ho for the deexcitation of ^{163}Dy has been calculated including the one- and two-hole excitations in Dy. The main improvements compared to Robertson [7] and to Carlson and Nestor [9] are: The two hole probabilities are calculated in the atoms Holmium and Dysprosium directly involved in electron capture, by which one wants to determine the neutrino mass. Robertson [7] used for electron capture in Z=67 Holmium results for Z=54 Xenon calculated by Carlson and Nestor [9].

The present work takes also into account selfconsistently in the relativistic Dirac-Hartree-Fock approach the different hole states in ^{163}Dy. So for each one hole state the remaining 65 electron wave functions are calculated selfconsistently and used to determine the two hole probabilities. The larger number of electrons in Dy than in Xe allows additional two hole states, which previously have not been included. The two hole probabilities in Dy calculated here are quite different from the probabilities of Robertson [7], Carlson and Nestor [9] calculated in Z=54 Xenon. To test the numerical results of this work three two-hole probabilities have also been calculated by hand.

The neutrino mass must be determined by a simultaneous fit together with the Q value and the properties of the relevant resonances (Assuming a Lorentzian profile these are positions, strengths and widths.) to the upper end of the spectrum. The finite neutrino mass provides at the upper end of the spectrum a characteristic deviation from the usual line shape, which can not be simulated by a resonance in Dy. This fingerprint close to the Q value should show up in the fit to the data. The finite experimental energy resolution has to be folded into the theoretical spectrum before one fits it to the data. Thus an excellent resolution of the measurement near the Q value is essential.

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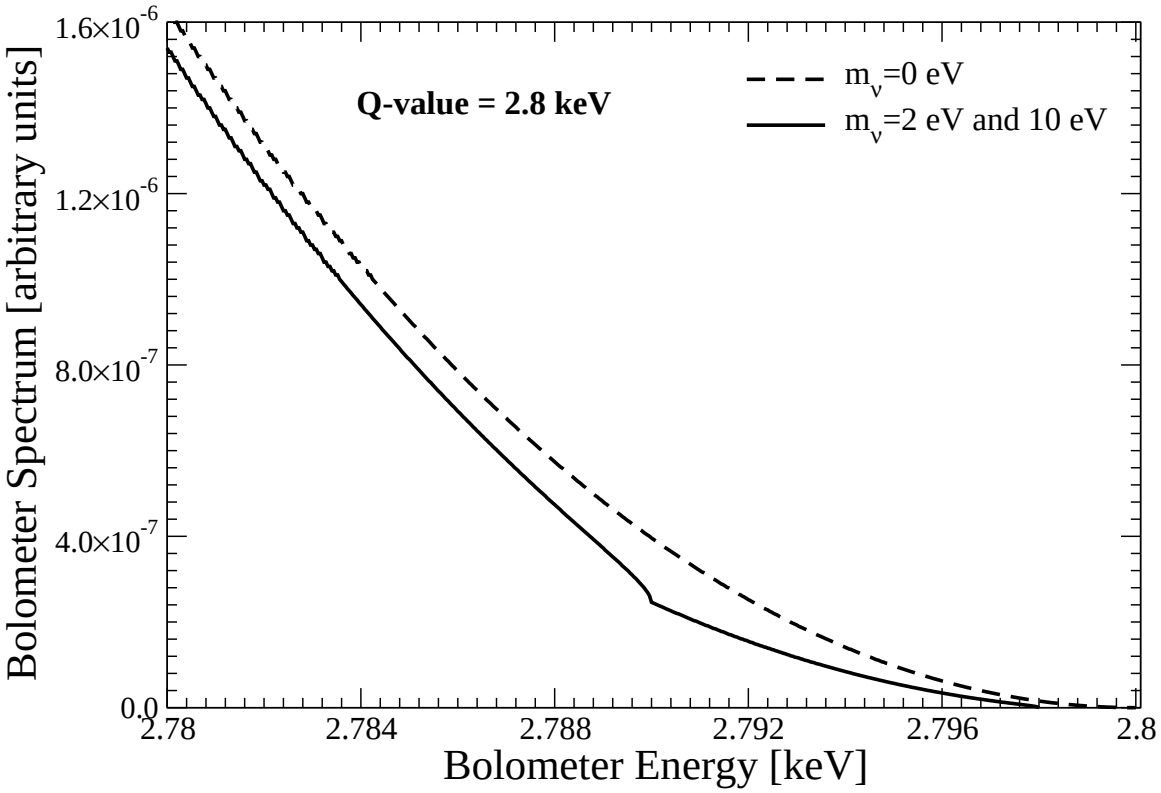

Figure 5: The upper 20 eV of the bolometer spectrum in ^{163}Dy for a neutrino with mass $m_\nu = 0\ eV$ (dashed line) and an electron neutrino, which is a mixture of two mass eigenstates with $m_\nu = 2\ eV$ *and* $m_\nu = 10\ eV$ (solid line) for the assumed Q-value = 2.8 keV. The mixing coefficients are adopted from [17] assuming only mixing of two neutrinos with probabilities of $U^2_{e,1}(2\ eV) = 0.636$ *and* $U^2_{e,2}(10\ eV) = 0.364$. The neutrino with $m_\nu = 0\ eV$ is assumed to have $U^2_{e,1} = 1.0$ and $U^2_{e,2} = 0.0$. The onset of the heavy neutrino of $m_\nu = 10\ eV$ at $(Q - 10)\ eV = 2.790\ keV$ can be seen in the theoretical spectrum. Finite experimental energy resolution will at least partially smear out this effect.